

Consistent Data Assimilation of Actinide Isotopes: ^{235}U and ^{239}Pu

G. Palmiotti
H. Hiruta
M. Salvatores

September 2011



The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

**Consistent Data Assimilation of Actinide Isotopes:
²³⁵U and ²³⁹Pu**

**G. Palmiotti
H. Hiruta
M. Salvatores**

September 2011

**Idaho National Laboratory
Idaho Falls, Idaho 83415**

<http://www.inl.gov>

**Prepared for the
U.S. Department of Energy
Office of Science
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517**

DISCLAIMER

This information was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness, of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. References herein to any specific commercial product, process, or service by trade name, trade mark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.

SUMMARY

In this annual report we illustrate the methodology of the consistent data assimilation that allows to use the information coming from integral experiments for improving the basic nuclear parameters used in cross section evaluation.

A series of integral experiments were analyzed using the EMPIRE evaluated files for ^{235}U , ^{238}U , and ^{239}Pu . In most cases the results have shown quite large worse results with respect to the corresponding existing evaluations available for ENDF/B-VII.

The observed discrepancies between calculated and experimental results were used in conjunction with the computed sensitivity coefficients and covariance matrix for nuclear parameters in a consistent data assimilation. Only the GODIVA and JEZEBEL experimental results were used, in order to exploit informations relative to the isotope of interest that are, in this particular case: ^{235}U and ^{239}Pu .

The results obtained by the consistent data assimilation indicate that with reasonable modifications (mostly within the initial standard deviation) it is possible to eliminate the original large discrepancies on the K_{eff} of the two critical configurations. However, some residual discrepancy remains for a few fission spectral indices that are, most likely, to be attributed to the detector cross sections.

CONTENTS

1.	INTRODUCTION	1
2.	THEORY	2
2.1	Consistent Data Assimilation Approach	2
2.2	Evaluation of Nuclear Physics Parameter Covariances	3
2.3	Evaluation Sensitivity Coefficients for Integral Experiments.....	3
2.4	Data Assimilation.....	3
3.	INTEGRAL EXPERIMENT ANALYSIS	4
3.1	Reflected and Unreflected Spheres	4
3.2	BIG TEN	5
3.3	ZPR6-6A/7 Assemblies.....	6
4.	^{239}Pu DATA ASSIMILATION.....	9
5.	^{235}U DATA ASSIMILATION.....	11
6.	CONCLUSIONS AND FUTURE WORK.....	13
	ACKNOWLEDGMENTS	13
7.	REFERENCES	14

1. INTRODUCTION

The major drawback of the classical adjustment method is the potential limitation of the domain of application of the adjusted data since adjustments are made on multigroup data, and the multigroup structure, the neutron spectrum used as weighting function and the code used to process the basic data file are significant constraints.

A new approach has been developed in order to adjust physical parameters and not multigroup nuclear data, the objective being now to correlate the uncertainties of some basic parameters that characterize the neutron cross section description, to the discrepancy between calculation and experimental value for a large number of clean, high accuracy integral experiments.

This new approach is the first attempt to build up a link between the wealth of precise integral experiments and basic theory of nuclear reactions. A large amount of exceptionally precise integral measurements has been accumulated over last 50 years. These experiments were driven by the necessities of nuclear applications but were never fully exploited for improving predictive power of nuclear reaction theory. Recent advances in nuclear reaction modeling and neutron transport calculations, combined with sensitivity analyses methods offer a reasonable possibility of de-convoluting results of the integral experiments in a way to obtain feedback on parameters entering nuclear reaction models. Essential ingredients of such a procedure will be covariances for model parameters and sensitivity matrices. The latter will provide direct link between reaction theory and integral experiments. By using integral reactor physics experiments (meter scale), information is propagated back to the nuclear level (femtometers) covering a range of more than 13 orders of magnitude.

The assimilation procedure results in more accurate and more reliable evaluated data files that will be of universal validity rather than tailored to a particular application. These files will naturally come with cross section covariances incorporating both microscopic and integral measurements as well as constraints imposed by the physics of nuclear reactions. Thus, these covariances will encompass the entire relevant knowledge available at the time of evaluation.

On the physics side, the assimilation improves knowledge of model parameters, increasing the predictive power of nuclear reaction theory and it would bring a new quality into nuclear data evaluation as well as refinements in nuclear reaction theory.

In this FY2011 report we deal with major actinides: ^{235}U , ^{238}U , and ^{239}Pu . First, we illustrate, again for clarity, the theoretical basis of the new approach. Then, we show the analysis of selected experiments that are relevant to the three isotopes that were the object of this year work. Next, we present a preliminary data assimilation for ^{235}U , and ^{239}Pu . For these two isotopes we used only a limited number of experiment for which the sensitivities are dominated by the isotope in question. In a next future, after we identify the most important nuclear parameters, and produce improved evaluated files for the two isotopes, we will include ^{238}U and the other experiments analyzed this year. Finally, we present some conclusions and directions for future work.

2. THEORY

The classical “statistical adjustment” techniques [1,2,3] provide adjusted multigroup nuclear data for applications, together with new, improved covariance data and reduced uncertainties for the required design parameters, in order to meet target accuracies.

One should, however, set up a strategy to cope with the drawbacks of the methodology, which are related to the energy group structure and energy weighting functions adopted in the adjustment.

In fact, the classical statistical adjustment method can be improved by “adjusting” reaction model parameters rather than multigroup nuclear data. The objective is to associate uncertainties of certain model parameters (such as those determining neutron resonances, optical model potentials, level densities, strength functions, etc.) and the uncertainties of theoretical nuclear reaction models themselves (such as optical model, compound nucleus, pre-equilibrium and fission models) with observed discrepancies between calculations and experimental values for a large number of integral experiments. The experiments should be clean (i.e., well documented with high QA standards) and high accuracy (i.e., with as low as possible experimental uncertainties and systematic errors), and carefully selected to provide complementary information on different features and phenomena, e.g., different average neutron spectrum energy, different adjoint flux shapes, different leakage components in the neutron balance, different isotopic mixtures and structural materials etc.

In the past, a few attempts were made [4,5,6] to apply a consistent approach for improving basic nuclear data, in particular to inelastic discrete levels and evaporation temperatures data of ^{56}Fe for shielding applications, and to resolved resonance parameters of actinides (e.g., Γ and total widths, peak positions etc.). This effort indicated the validity of the approach but also challenges to be overcome for its practical application. This was mainly related to the way of getting the sensitivity coefficients and to the need of reliable covariance information.

2.1 Consistent Data Assimilation Approach

The Consistent Data Assimilation methodology allows overcoming both difficulties, using the approach that involves the following steps:

- Selection of the appropriate reaction mechanisms along with the respective model parameters to reproduce adopted microscopic cross section measurements with the EMPIRE [7] code calculations. Use of coupled channels, quantum-mechanical pre-equilibrium theories, and advanced statistical model accounting for width fluctuations and full gamma cascade ensure state of the art modelling of all relevant reaction mechanisms.
- Determination of covariances matrices for the set of nuclear reaction model parameters obtained in the previous step. This is achieved by combining initial estimates of parameter uncertainties, with uncertainties/covariances for the adopted experimental data through the KALMAN [8] code. This way, the resulting parameter covariances will contain constraints imposed by nuclear reaction theory and microscopic experiments. Several parameters have been considered, including resonance parameters for a few dominating resonances, optical model parameters for neutrons, level density parameters for all nuclei involved in the reaction, parameters entering pre-equilibrium models, and parameters determining gamma-strength functions.
- Sensitivity of cross sections to the perturbation of the above mentioned reaction model parameters are calculated with the EMPIRE code.
- Use of the adjoint technique to evaluate sensitivity coefficients of integral reactor parameters to the cross section variations, as described in the previous step. To perform this task, the ERANOS code system [9] that computes sensitivity coefficients based on generalized perturbation theory is employed.
- Performing analysis of selected experiments using the best calculation tools available (in general Monte Carlo codes like MCNP).
- Performing consistent data assimilation on basic nuclear parameters using integral experiment analysis with best methodology available to provide discrepancies between calculation and measured quantities. After the C/E's are available, they are used together with the sensitivity coefficients coming from the previous step in a data assimilation code.
- Constructing new ENDF/B type data files based on modified reaction theory parameters for use by neutronic designers.

2.2 Evaluation of Nuclear Physics Parameter Covariances

As indicated in the outline of the methodology, the first step is to provide estimated range of variation of nuclear physics parameters, including their covariance data. To this end the code EMPIRE [7] coupled to the KALMAN [8] code is employed.

KALMAN code is an implementation of the Kalman filter technique based on minimum variance estimation. It naturally combines covariances of model parameters, of experimental data and of cross sections. This universality is a major advantage of the method. KALMAN uses measurements along with their uncertainties to constrain covariances of the model parameters via the sensitivity matrix. Then, the final cross section covariances can be calculated from the updated covariances for model parameters. This procedure consistently accounts for the experimental uncertainties and the uncertainties of the nuclear physics parameters. We emphasize that under the term 'reaction model' we mean also the resonance region described by models such as the Multi-Level Breit-Wigner formalism.

2.3 Evaluation Sensitivity Coefficients for Integral Experiments

In order to evaluate the sensitivity coefficients of the nuclear parameters to the integral parameters measured in a reactor physics experiment, a folding procedure is applied, where the sensitivity calculated by EMPIRE, are folded with those calculated by ERANOS (i.e multigroup cross section sensitivity coefficient to integral parameters).

Following this procedure, the sensitivities of integral experiments to nuclear parameters p_k are defined as:

$$\frac{\Delta R}{\Delta p_k} = \sum_j \frac{\Delta R}{\Delta \sigma_j} \times \frac{\Delta \sigma_j}{\Delta p_k} \quad (1)$$

where R is an integral reactor physics parameter (e. g. K_{eff} , reaction rates, reactivity coefficient, etc.), and σ_j a multigroup cross section (the j index accounts for isotope, cross section type and energy group).

In general to compute σ_j one can use a) EMPIRE with an appropriate set of parameters p_k to generate first b) an ENDF/B file for that specific isotope and successively, c) to use NJOY, to obtain multi-group cross sections.

As specified in the previous section, one can compute the variation of the cross sections $\Delta \sigma_j$ resulting from a variation of each parameter p_k variation.

Specifically, the procedure would consist in the generation of the $\Delta \sigma_j$ corresponding to fixed, well chosen variations of each p_k taken separately and therefore generating the $\frac{\Delta \sigma_j}{\Delta p_k}$. Following each EMPIRE calculation, an

ENDF/B file for the isotope under consideration is generated and a subsequent run of NJOY on this file generates multigroup cross sections in the same energy structure used for the computation of the reactor physics integral parameters. The multigroup cross section variations associated to the individual fundamental parameter that has been varied in the corresponding EMPIRE calculation are readily computed by difference with the reference NJOY calculation for the isotope under consideration.

In parallel, the cross section sensitivity coefficients to integral parameter R:

$$\frac{\Delta R}{\Delta \sigma_j}$$

are provided, using the standard Generalized Perturbation Theory in the ERANOS code system [9].

Folding the two contributions (from EMPIRE and ERANOS) one obtains the sensitivity coefficients of the nuclear physics parameters to the integral measured parameters, see Eq. (1).

2.4 Data Assimilation

Finally as far as data adjustment (or data "assimilation") the methodology makes use of:
 quantified uncertainties and associated variance-covariance data;
 well documented, high accuracy and "representative" integral experiments;
 sensitivity coefficients for a variety of integral parameters.

A statistical adjustment is performed using these quantities. Formulation is given in reference [1].

3. INTEGRAL EXPERIMENT ANALYSIS

The files containing the evaluation by BNL of ^{235}U , ^{238}U , and ^{239}Pu using the EMPIRE code were used to analyze a set of experiments intended for a future consistent data assimilation. The selected experiments [10] include: JEZEBEL, GODIVA, and FLATTOPS bare critical reflected and unreflected spheres, BIG TEN assembly which is entirely fuelled with ^{235}U and contains minor amount of structural materials, and the full-core configurations of ZPR6-6A and ZPR6-7.

3.1 Reflected and Unreflected Spheres

Selected critical experiments with reflected and unreflected spheres were analyzed using simplified geometry. Those are:

- ^{239}Pu JEZEBEL: Bare unreflected sphere of Pu-239 metal (4.5 at.% Pu-240, 1.02 wt.% Ga),
- ^{240}Pu JEZEBEL: Bare unreflected sphere of Pu-239 metal (20.1 at.% Pu-240, 1.01 wt.% Ga),
- GODIVA: Bare unreflected sphere of highly enriched uranium,
- FLATTOP-Pu: Plutonium sphere reflected by normal uranium,
- FLATTOP-25: U-235 sphere reflected by normal uranium.

Tables 1-3 show calculated k_{eff} and C/E ratios of spectral indices for each sphere and compares to those obtained with ENDF/B-VII.0. The spectral indices were calculated by defining a point detector at the center of sphere. As seen in Table 1, k_{eff} 's calculated with ENDF/B-VII.0 are generally closer to the reference values than those with EMPIRE cross sections. However, spectral indices have almost the same quality in both EMPIRE and ENDF/B-VII.0.

Table 1: k_{eff} results for each sphere (experimental $k_{eff}=1.0(\pm 100\sim 300\text{pcm})$).

Experiment	EMPIRE ($\pm\text{pcm}$)	ENDF/B-VII.0 ($\pm\text{pcm}$)
JEZEBEL-239	0.98567 (± 8)	0.99986 (± 9)
GODIVA	0.99072 (± 9)	0.99983 (± 9)
FLATTOP-Pu	0.98838 (± 18)	1.00097 (± 18)
FLATTOP-25	1.00182 (± 17)	1.00217 (± 17)

Table 2: C/E ratio of spectral indices at the center of JEZEBEL-239 and GODIVA

	JEZEBEL-239		GODIVA	
	EMPIRE	ENDF/B-VII.0	EMPIRE	ENDF/B-VII.0
$\sigma_f(^{238}\text{U})/\sigma_f(^{235}\text{U})$	0.956 \pm 0.009	0.974 \pm 0.009	1.053 \pm 0.013	0.954 \pm 0.012
$\sigma_f(^{233}\text{U})/\sigma_f(^{235}\text{U})$	1.000 \pm 0.017	0.986 \pm 0.017	0.996 \pm 0.019	0.987 \pm 0.019
$\sigma_f(^{237}\text{Np})/\sigma_f(^{235}\text{U})$	0.999 \pm 0.017	1.009 \pm 0.017	1.070 \pm 0.017	0.990 \pm 0.016
$\sigma_f(^{239}\text{Pu})/\sigma_f(^{235}\text{U})$	0.971 \pm 0.020	0.984 \pm 0.020	0.992 \pm 0.018	0.986 \pm 0.018

Table 3: C/E ratio of spectral indices at the center of FLATTOPs

	FLATTOP-Pu		FLATTOP-25	
	EMPIRE	ENDF/B-VII.0	EMPIRE	ENDF/B-VII.0
$\sigma_f(^{238}\text{U})/\sigma_f(^{235}\text{U})$	0.9705±0.0110	0.982±0.013	1.056±0.012	0.966±0.003
$\sigma_f(^{233}\text{U})/\sigma_f(^{235}\text{U})$			0.983±0.003	0.975±0.011
$\sigma_f(^{237}\text{Np})/\sigma_f(^{235}\text{U})$	0.9915±0.0140	0.996±0.014	1.059±0.014	0.988±0.013
$\sigma_f(^{239}\text{Pu})/\sigma_f(^{235}\text{U})$			0.986±0.009	0.982±0.009

3.2 BIG TEN

The Big Ten assembly is a large, mixed-uranium-metal cylindrical core fueled by ²³⁵U (10% average enrichment) surrounded by a thick ²³⁸U reflector. The detailed Big Ten model represents the essential structural detail in the assembly with some approximations in boundaries. We compare both k_{eff} and spectral indices. During the actual measurement, sample specimens were traversed along the sample transfer bar through the geometric center of Big Ten assembly (see Figure 1). Therefore, in our MCNP5 model, we defined a point detector along this sample transfer bar for calculations of spectral indices at the center of the core.

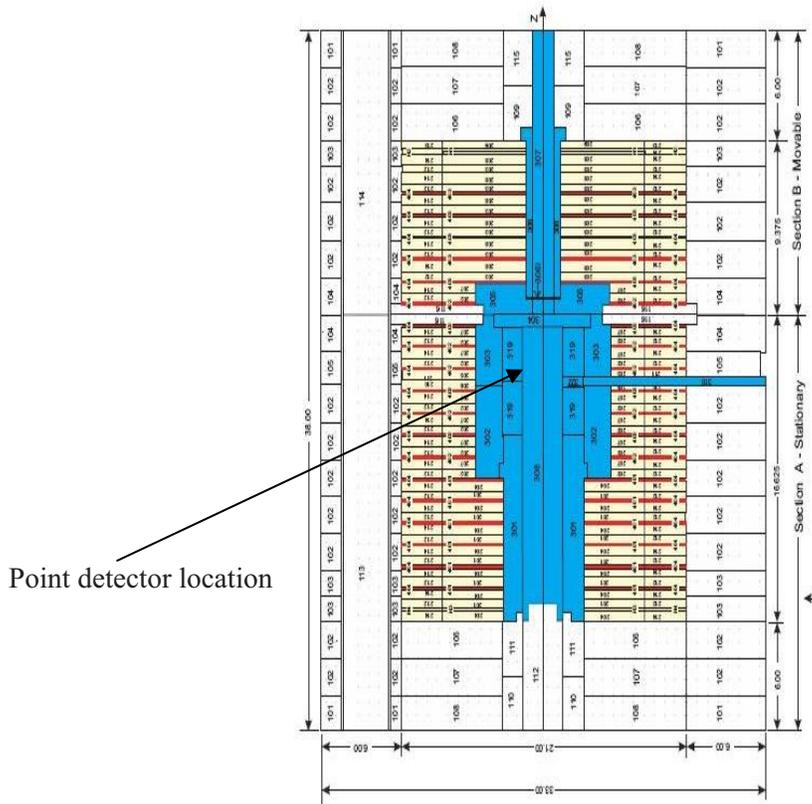


Figure 1: Detailed schematic of Big Ten (from IHECSBE DVD [1]).

Tables 4 and 5 show calculated k_{eff} and C/E ratios of spectral indices of Big Ten model, respectively. Here, again k_{eff} obtained with ENDF/B-VII.0 is much closer to the reference value than the one obtained with EMPIRE cross sections. For spectral indices, a slight improvement can be observed in the index $\sigma_f(^{238}\text{U})/\sigma_f(^{235}\text{U})$ with EMPIRE cross sections. However, the qualities of the rest of indices are mostly the same as those with ENDF/B-VII.0.

Table 4: k_{eff} results for BIG TEN models

	Reference	EMPIRE	ENDF/B-VII.0
k_{eff}	1.0045±0.0007	1.0071±0.0001	1.0045±0.0001

Table 5: Spectral indices at the center of Big Ten Assembly

Spectral Index	Experimental Result	C/E (EMPIRE)	C/E (ENDF/B-VII.0)
$\sigma_f(^{238}\text{U})/\sigma_f(^{235}\text{U})$	0.03739±0.00034	1.0008±0.0147	0.9468±0.0137
$\sigma_f(^{237}\text{Np})/\sigma_f(^{235}\text{U})$	0.3223±0.003	1.0392±0.0109	0.9668±0.0101
$\sigma_f(^{239}\text{Pu})/\sigma_f(^{235}\text{U})$	1.1936±0.0084	0.9808±0.0075	0.9744±0.0075
$\sigma_f(^{233}\text{U})/\sigma_f(^{235}\text{U})$	1.580±0.030	0.9759±0.0188	0.9777±0.0188
$\sigma_{n,\gamma}(^{238}\text{U})/\sigma_{n,\gamma}(^{235}\text{U})$	0.110±0.003	1.0315±0.0283	0.9709±0.0266

3.3 ZPR6-6A/7 Assemblies

ZPR 6 is a large cylindrical assembly surrounded by a thick depleted-uranium reflector. The main difference between Assemblies 6A and 7 is that the Assembly 6A is fueled by uranium oxide while Assembly 7 uses mixed Pu-U oxide.

There were two principal core configuration established for the ZPR6-7 program. Those were the uniform core loading and high ^{240}Pu -zone core loading [1]. The former had a relatively uniform core composition. A central zone of 61 matrix locations in each half of the assembly was defined as the exact core. This exact core region had the same unit cell and the same average composition as the outer core, but the plates used in the exact core were those for which knowledge of material properties was most precise. The latter configuration was a variant of the uniform core. The plutonium in the standard Pu-U-Mo fuel plates used in the uniform core contains 11% ^{240}Pu . The high ^{240}Pu zone was built by replacing all of the Pu-U-Mo plates in the exact core region of the uniform core with Pu-U-Mo plates containing 27% ^{240}Pu in the plutonium component. The high ^{240}Pu zone had a composition closer to that in an LMFBR core with high burnup [1].

The analyses of these assemblies were performed using detailed geometry models (Figures 2 and 3). Table 6 shows calculated k_{eff} 's based on these detailed ZPR6 models. The k_{eff} 's obtained with EMPIRE cross sections have almost the similar quality as those with ENDF/B-VII.0.

Table 6: k_{eff} results for ZPR 6

	ZPR 6-6A	ZPR 6-7	ZPR 6-7 High- ^{240}Pu
Reference	1.00164 ± 0.00005	1.00051 ± 0.00087	1.0008 ± 0.0009
EMPIRE	1.0009 ± 0.0001	1.0084 ± 0.0001	1.0073 ± 0.0001
ENDF/B-VII.0	1.0005 ± 0.0001	0.9980 ± 0.0001	0.9924 ± 0.0001

The cell average spectral indices in ZPR6-7 were measured at the 2×2×2 inch box in the central drawer along the core mid-plane. The configuration of the central drawer is shown in Figure 4. The cell average spectral indices were calculated based on the atomic density weighted approach given by:

$$\text{Reaction rate of Isotope } n = \frac{\sum_{i=1}^3 R_i^n A_i^n}{\sum_{i=1}^3 A_i^n}$$

where R_i^n , and A_i^n refer to reaction rate and atomic density of Isotope n at Fuel plate i , respectively. Calculated results are compared in Table 7. Both types of cross sections produced similar quality of solutions.

Table 7: Spectral indices at the central 2×2×2 inch box in the uniform core loading ZPR6-7

Spectral Index	Experiment	C/E (Empire)	C/E (ENDF/B-VII.0)
$\sigma_f(^{235}\text{U}) / \sigma_f(^{239}\text{Pu})$	1.0599 ± 0.0223	1.0241 ± 0.0224	1.0376 ± 0.0227
$\sigma_f(^{238}\text{U}) / \sigma_f(^{235}\text{U})$	0.0223 ± 0.0007	1.0045 ± 0.0328	1.0045 ± 0.0328
$\sigma_f(^{238}\text{U}) / \sigma_f(^{239}\text{Pu})$	0.0233 ± 0.0007	1.0385 ± 0.0322	1.0601 ± 0.0344
$\sigma_{n,\gamma}(^{238}\text{U}) / \sigma_f(^{235}\text{U})$	0.1323 ± 0.0032	1.0340 ± 0.0257	1.0098 ± 0.0252
$\sigma_{n,\gamma}(^{238}\text{U}) / \sigma_f(^{239}\text{Pu})$	0.1399 ± 0.0032	1.0585 ± 0.0252	1.0500 ± 0.0251
$\sigma_{n,\gamma}(^{238}\text{U}) / \sigma_f(^{238}\text{U})$	5.8903 ± 0.1897	1.0416 ± 0.0351	1.0111 ± 0.0342

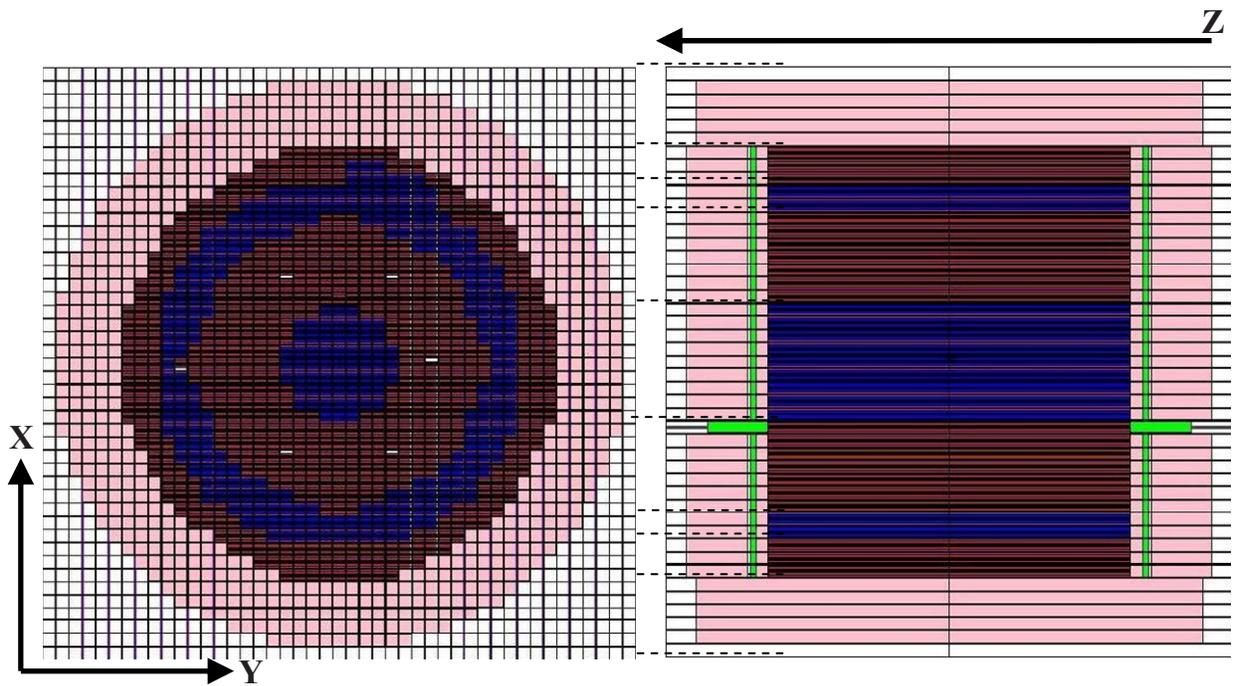


Figure 2: Cross sectional view of the detailed ZPR6-6A MCNP model

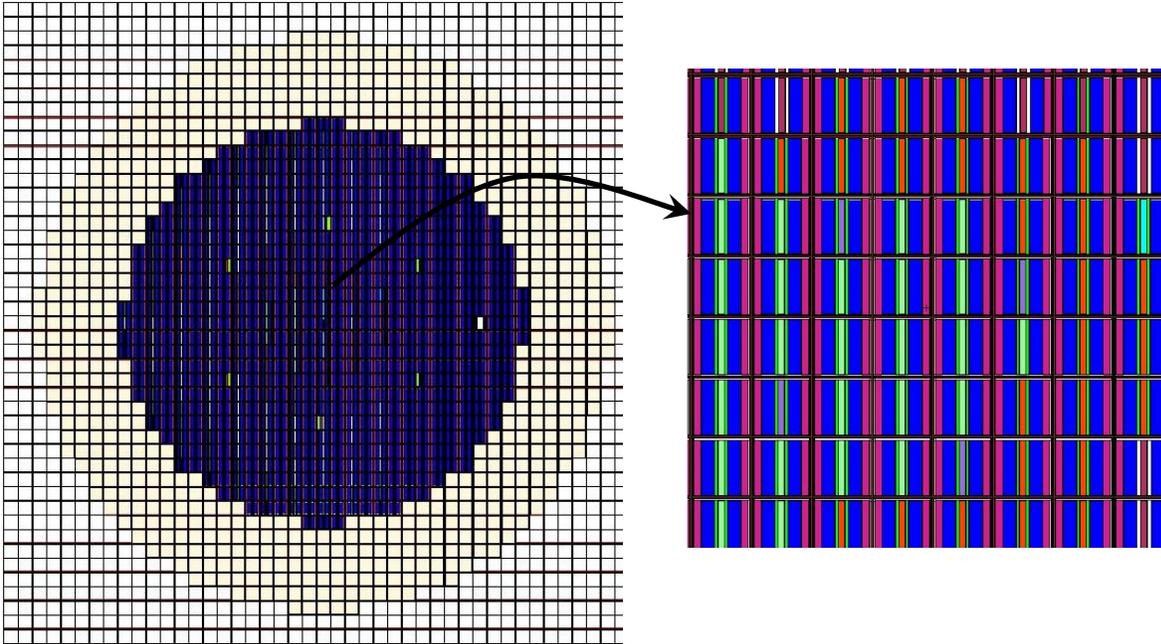


Figure 3: Radial cross sectional view of ZPR6-7 with the high ^{240}Pu zone model

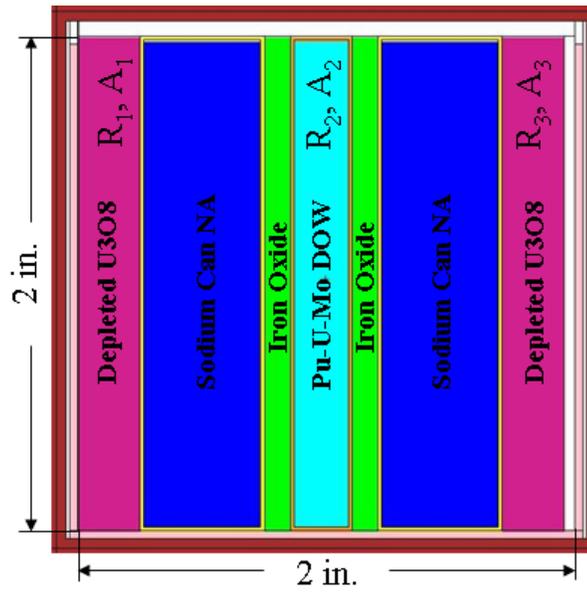


Figure 4: ZPR6-7 central drawer.

4. ^{239}Pu DATA ASSIMILATION

For this case we have used the experiments performed at LANL sphere JEZEBEL. The integral parameters considered are the critical mass (K_{eff}), and the fission spectral indices, with respect of ^{235}U , ^{238}U , ^{239}Pu , ^{237}Np , and ^{233}U . The critical mass is directly dependent from the cross sections of ^{239}Pu , while the spectral indices have an indirect (spectral) dependence from ^{239}Pu . A total of 40 nuclear parameters were used in EMPIRE for characterizing the evaluation of the ^{239}Pu cross sections.

BNL provided the covariance matrix of these parameters as well the sensitivity of them in terms of multigroup cross sections. The classical 33 group structure, used mostly for fast reactors and reported in Table 8, was adopted. The ERANOS code [9] was used to calculate the multigroup sensitivity coefficients to the five integral parameters previously indicated.

With these two sets the sensitivity of the nuclear parameters to the measured quantities was calculated following Eq. (1). Subsequently, this set of sensitivity coefficients was used together with the calculated C/E (shown in the previous chapter) for performing a statistical adjustment. Table 9 shows the C/E before and after adjustment with related uncertainties.

Table 8. Multigroup energy structure (eV).

Group	Up Ener.	Group	Up Ener.	Group	Up Ener.
1	$1.96 \cdot 10^7$	12	$6.74 \cdot 10^4$	23	$3.04 \cdot 10^2$
2	$1.00 \cdot 10^7$	13	$4.09 \cdot 10^4$	24	$1.49 \cdot 10^2$
3	$6.07 \cdot 10^6$	14	$2.48 \cdot 10^4$	25	$9.17 \cdot 10^1$
4	$3.68 \cdot 10^6$	15	$1.50 \cdot 10^4$	26	$6.79 \cdot 10^1$
5	$2.23 \cdot 10^6$	16	$9.12 \cdot 10^3$	27	$4.02 \cdot 10^1$
6	$1.35 \cdot 10^6$	17	$5.53 \cdot 10^3$	28	$2.26 \cdot 10^1$
7	$8.21 \cdot 10^5$	18	$3.35 \cdot 10^3$	29	$1.37 \cdot 10^1$
8	$4.98 \cdot 10^5$	19	$2.03 \cdot 10^3$	30	$8.32 \cdot 10^0$
9	$3.02 \cdot 10^5$	20	$1.23 \cdot 10^3$	31	$4.00 \cdot 10^0$
10	$1.83 \cdot 10^5$	21	$7.49 \cdot 10^2$	32	$5.40 \cdot 10^{-1}$
11	$1.11 \cdot 10^5$	22	$4.54 \cdot 10^2$	33	$1.00 \cdot 10^{-1}$

Table 9. Old and new C/E before and after adjustment for JEZEBEL experiments

Experiment	old C/E $\pm \sigma$	new C/E $\pm \sigma$
K_{eff}	0.9857 ± 0.002	0.9998 ± 0.002
Fis. ^{238}U /Fis. ^{235}U	0.9561 ± 0.009	0.9598 ± 0.002
Fis. ^{239}Pu /Fis. ^{235}U	0.9708 ± 0.020	0.9917 ± 0.003
Fis. ^{237}Np /Fis. ^{235}U	0.9988 ± 0.017	1.0010 ± 0.001
Fis. ^{233}U /Fis. ^{235}U	1.0003 ± 0.017	1.0002 ± 0.001

A significant improvement was obtained on the discrepancies on K_{eff} and the fission spectral index of ^{239}Pu , while that of the fission spectral index of ^{238}U stays essential the same after adjustment. The remaining two fission spectral indices were already in good agreement and do not change significantly. The two improved integral parameters are directly related to the ^{239}Pu fission cross sections, and, therefore, one should expect such amelioration. For the ^{238}U spectral index it is likely that an improvement would be obtained when we take into account the dependence from the ^{238}U fission cross section.

The χ^2 test after adjustment provided a normalized (to the number of degrees of freedom) value of 5.03; however, most (4.6) of the contribution to this value is coming from the ^{238}U spectral index integral parameter. Table 10 shows the obtained parameter variations before and after the data assimilation for the parameters that mostly affect the assimilation.

Table 10 ^{239}Pu parameter variations and standard deviations obtained by data assimilation.

Parameter	Variation (%)	Init. Stand. Dev. (%)	Final Stand. Dev. (%)
VA000000 ^{a)}	-0.141	0.134	0.121
FUSRED000000 ^{b)}	0.432	0.951	0.612
LDSHIF000100 ^{c)}	0.299	0.705	0.692
DELTA000000 ^{d)}	-0.120	0.671	0.668
ATILNO000100 ^{e)}	-0.076	0.965	0.958
VB000000 ^{f)}	-0.079	0.480	0.479
ATLATF000000 ^{g)}	0.128	1.240	1.239
TOTRED000000 ^{h)}	-0.081	0.918	0.815
HA000000 ⁱ⁾	-0.155	0.474	0.471

^{a)} Height of the first fission barrier hump in ^{240}Pu , ^{b)} Factor multiplying the reaction (fusion, absorption, compound nucleus formation) cross section, ^{c)} Shift of the level densities in target at the point they reach discrete levels (LDSHIFT - 1) MeV, ^{d)} Pairing energy used in the level densities at the saddle point in ^{240}Pu , ^{e)} Factor multiplying asymptotic level density parameter in the target, ^{f)} Height of the second fission barrier hump in ^{240}Pu , ^{g)} Factor multiplying asymptotic level density parameter at saddle point in ^{240}Pu , ^{h)} Factor multiplying total cross section, ⁱ⁾ Width of the first fission barrier hump in ^{239}Pu .

One can notice that only the VA000000 parameter variation indicated by the data assimilation slightly exceeds the 1σ initial uncertainty, while the other variations stay within that range. In Table 11 we report the contribution of the parameter variations of Table 10 to the relative change of the C/E of the JEZEBEL K_{eff} .

Table 11 Contribution of the parameter variation to the relative change of the C/E of the JEZEBEL K_{eff} .

Parameter	Variation (pcm)
VA000000	630
FUSRED000000	298
LDSHIF000100	223
DELTA000000	184
VB000000	67
ATLATF000000	48
ATILNO000100	31
HA000000	-29
TOTRED000000	-4
Total	1435

It is interesting to note that the new standard deviations of Table 10 obtained after the data assimilation produce a reduction of the evaluated uncertainty of the JEZEBEL K_{eff} of 18.7% mostly coming from the fission cross section contribution. This is already an indication of the potential gain, in terms of uncertainty reduction, that the data assimilation can produce. One should expect more reductions when other integral experiments are included in the data assimilation process.

5. ^{235}U DATA ASSIMILATION

The data assimilation process was repeated for the ^{235}U . We used the experimental data of the LANL sphere GODIVA. The integral parameters considered are the critical mass (K_{eff}), and the fission spectral indices, with respect of ^{235}U , ^{238}U , ^{239}Pu , ^{237}Np , and ^{233}U . A total of 52 nuclear parameters were used in EMPIRE for characterizing the evaluation of the ^{235}U cross sections.

BNL provided the covariance matrix of these parameters as well the sensitivity of them in terms of multigroup cross sections, and as before for the ^{239}Pu a statistical adjustment was carried out. Table 12 shows the C/E before and after adjustment with related uncertainties.

Table 12. Old and new C/E before and after adjustment for GODIVA experiments

Experiment	old C/E $\pm \sigma$	new C/E $\pm \sigma$
K_{eff}	0.9907 \pm 0.002	1.0010 \pm 0.002
Fis. ^{238}U /Fis. ^{235}U	1.0527 \pm 0.013	1.0357 \pm 0.004
Fis. ^{239}Pu /Fis. ^{235}U	0.9917 \pm 0.018	0.9771 \pm 0.003
Fis. ^{237}Np /Fis. ^{235}U	1.0703 \pm 0.017	1.0536 \pm 0.003
Fis. ^{233}U /Fis. ^{235}U	0.9964 \pm 0.019	0.9820 \pm 0.004

A significant improvement was obtained on the discrepancies on K_{eff} while for the fission spectral indices improvements (but still not good agreement with experimental values) are observed for the ^{238}U and ^{237}Np , while for ^{239}Pu and ^{233}U a certain degradation is observed.

The χ^2 test after adjustment provided a normalized (to the number of degrees of freedom) value of 4.05; with major contributions coming from the ^{238}U (contribution of 2.01) and ^{237}Np (contribution of 2.36) spectral index integral parameters. Table 13 shows the obtained parameter variations before and after the data assimilation for the parameters that mostly affect the assimilation.

Table 13 ^{235}U parameter variations and standard deviations obtained by data assimilation.

Parameter	Variation (%)	Init. Stand. Dev. (%)	Final Stand. Dev. (%)
FUSRED000000 ^{a)}	1.402	1.257	0.878
TOTRED000000 ^{b)}	0.461	0.966	0.917
ATILNO000000 ^{c)}	-0.236	0.950	0.946
DELTA000000 ^{d)}	-0.025	0.649	0.621
VB000000 ^{e)}	-0.006	0.133	0.118
UOMPVV000101 ^{f)}	0.033	0.116	0.116
UOMPRS000101 ^{g)}	0.072	0.834	0.834
UOMPWS000101 ^{h)}	-0.110	2.023	2.022
TUNE000000 ⁱ⁾	-0.099	1.908	1.908

^{a)} Factor multiplying the reaction (fusion, absorption, compound nucleus formation) cross section, ^{b)} Factor multiplying total cross section, ^{c)} Asymptotic level density parameter in Compound Nucleus, ^{d)} Pairing energy in the level densities at the saddle point in Compound Nucleus (first chance fission), ^{e)} Height of the second hump in the fission barrier in Compound Nucleus, ^{f)} Real depth of the Optical Model potential for n + target, ^{g)} Surface imaginary Optical Model potential radius for n + target, ^{h)} Surface imaginary Optical Model potential depth for n + target, ⁱ⁾ Factor on the gamma emission width in Compound Nucleus (scales capture).

Only the FUSRED000000 parameter variation indicated by the data assimilation slightly exceeds the 1σ initial uncertainty, while the other variations stay within that range. In Table 14 we report the contribution of the parameter variations of Table 13 to the relative change of the C/E of the GODIVA K_{eff} . The largest, dominating, contribution is provided by the FUSRED000000 parameter.

Table 41 Contribution of the parameter variation to the relative change of the C/E of the GODIVA K_{eff} .

Parameter	Variation (pcm)
FUSRED000000	867
TOTRED000000	66
ATILNO000000	43
DELTA000000	31
VB000000	29
UOMPVV000101	-18
UOMPRS000101	6
UOMPWS000101	-6
TUNE000000	6
Total	1038

As for ^{239}Pu we have applied the new standard deviations obtained by the data assimilation to reevaluate the uncertainty of the GODIVA K_{eff} . A reduction of 13.8% was observed, and again mostly coming from the fission cross section contribution.

6. CONCLUSIONS AND FUTURE WORK

In this annual report we have again illustrated the methodology of the consistent data assimilation that allows to use the information coming from integral experiments for improving the basic nuclear parameters used in cross section evaluation.

A series of integral experiments were analyzed using the EMPIRE evaluated files for ^{235}U , ^{238}U , and ^{239}Pu . In most cases the results have shown quite large worse results with respect to the corresponding existing evaluations available for ENDF/B-VII.

The observed discrepancies between calculated and experimental results were used in conjunction with the computed sensitivity coefficients and covariance matrix for nuclear parameters in a consistent data assimilation. Only the GODIVA and JEZEBEL experimental results were used, in order to exploit informations relative to the isotope of interest that are, in this particular case: ^{235}U and ^{239}Pu .

The results obtained by the consistent data assimilation indicate that with reasonable modifications (mostly within the initial standard deviation) it is possible to eliminate the original large discrepancies on the K_{eff} of the two critical configurations. However, some residual discrepancy remains for a few fission spectral indices that are, most likely, to be attributed to the detector cross sections.

In the future, a most comprehensive data assimilation, that will include all experiment analyzed, as well the ^{238}U isotope will be performed.

Next fiscal year the consistent data assimilation will be extended to a minor Pu isotope (^{242}Pu) and a fission product (^{105}Pd) making use of experimental information coming from analyzing irradiation experiments.

ACKNOWLEDGMENTS

The work performed and reported in this document is supported by a project funded by the DOE Office of Science in the framework of the Recovery Act (ARRA).

7. REFERENCES

1. Gandini, M. Petilli, "AMARA: A Code Using the Lagrange Multipliers Methods of Nuclear Data Adjustment," RT/FI(73)39, Comitato Nazionale per l'Energia Nucleare, Italy (1973).
2. Gandini, "Uncertainty Analysis and Experimental Data Transposition Methods in Uncertainty Analysis," Y. Ronen, Editor, CRC Press, 1988.
3. M. Salvatores, G. Aliberti, G. Palmiotti, "Nuclear Data Validation and Fast Reactor Design Performances Uncertainty Reduction," Trans. ANS Meeting, **96**, 519, Boston, Massachusetts, June 22-26, 2007.
4. A. Gandini, M. Salvatores, "Nuclear data and Integral Measurements Correlation for Fast reactors-Part 3: The Consistent Method", RT/FI(74)3, Comitato per l'Energia Nucleare (1974)
5. D'Angelo, A. Oliva, G. Palmiotti, M. Salvatores, and S. Zero, "Consistent Utilization of Shielding Benchmark Experiments," *Nuclear Science Engineering* **65**, 477 (1978).
6. M. Salvatores, and G. Palmiotti, et al. "Resonance Parameter Data Uncertainty Effects on Integral Characteristics of Fast Reactors," IAEA Specialist's Meeting on Resonance Parameters, Vienna, 28 September - 2 October, 1981.
7. M. Herman, R. Capote, B.V. Carlson, P. Oblozinsky et al, "EMPIRE: Nuclear Reaction Model Code System for Data Evaluation", *Nucl. Data Sheets* **108** (2007) 2655-2715
8. T. KAWANO and K. SHIBATA, "Covariance Evaluation System," JAERI-Data/Code 97-037, Japan Atomic Energy Research Institute (1997) (n Japanese).
9. G. Rimpault, et al., "The ERANOS Code and Data System for Fast Reactor Neutronic Analyses," Proc. Physor 2002 Conference, Seoul (Korea), October 2002.
10. International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC(95)03, September 2008 Edition.